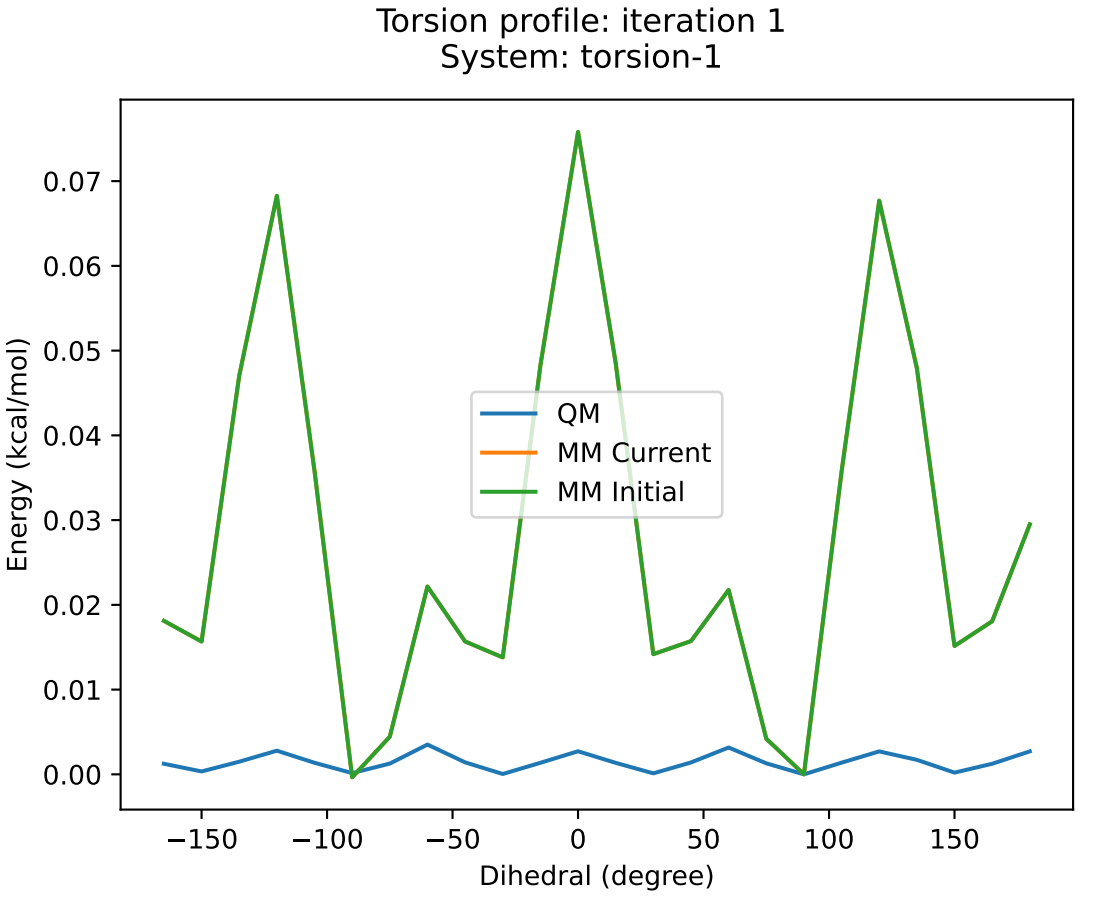
Torsion profile: iteration 1
System: torsion-1
Energy (kcal/mol)
0.00
0.01
0.02
0.03
0.04
0.05
0.06
0.07
−150
−100
−50
0
50
100
150
Dihedral (degree)
QM
MM Current
MM Initial